

# Coupling of two Dirac particles

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A study of the formation of excitons as a problem of two Dirac particles in a gapped graphene layer and in two gapped graphene layers separated by a dielectric is presented. In the low-energy limit the separation of the center-of-mass and relative motions is obtained. Analytical solutions for the wave function and energy dispersion for both cases when electron and hole interact via a Coulomb potential are found. It is shown that the energy spectrum and the effective exciton mass are functions of the energy gaps as well as interlayer separation in case of two layer gapped graphene.

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## I. INTRODUCTION

The exciton formed by an electron and a hole is one of the very important objects in both experimental and theoretical physics of semiconductor heterostructures and graphene. The study of the excitonic system and its properties is necessary because of potential applications in electronics and photonics, including, design of thresholdless lasers, optical computing and quantum computing [1–8]. From the theoretical point of view, an exciton is a two-body system and to address the problem we have to solve a two-body problem in semiconductor heterostructures or graphene. Let us mention that the problem of the interaction between two particles is very important for the deep analysis of the many-body physics in excitonic system. The analysis of the spectrum of collective excitations necessary to study such many-body phenomena in the excitonic system as Bose-Einstein condensation and superfluidity [9] requires the solution of two-body problem for a single exciton. The temperature of Kosterlitz-Thouless phase transition corresponding to the superfluidity depends on the density of the superfluid component [10]. This density of the superfluid component is defined by the two-particle Green function of weakly interacting excitons. The problem to find the two-particle Green function of the interacting excitons requires one-particle Green function of non-interacting excitons, which is defined by the wave function and energy dispersion of a single exciton [11]. The collective properties and superfluidity of excitons and polaritons in gapped graphene have been studied in Refs. 12, 13. Therefore, it is of fundamental and practical interest to focus on solution of two-body problem in semiconductor heterostructures and graphene. Finding solution of two-body problem in gapped graphene layers is the subject of this Paper.

To describe the formation of an exciton in semiconductor heterostructures like quantum wells the standard quantum mechanical approach is used based on Schrödinger equation. In this case the two-body problem with a scalar action-at-a-distance inter-particle potentials is completely understood and developed both in configuration or momentum three dimensional as well as two dimensional (2D) spaces [14–16]. The notions of absolute time and absolute space allow us to describe the two particles of masses  $m_1$  and  $m_2$  with Euclidean position vectors  $\mathbf{r}_1$  and  $\mathbf{r}_2$ , and momenta  $\mathbf{p}_1$  and  $\mathbf{p}_2$  in an inertial frame. It is well known [14] that in the covariant mechanics, the most straightforward solution of the classical problem with scalar interaction is obtained by a transformation from the individual particle coordinates  $\mathbf{r}_1$ ,  $\mathbf{r}_2$  and  $\mathbf{p}_1$ ,  $\mathbf{p}_2$  to the covariant center-of-mass and relative coordinates. Using canonical transformation

$$\mathbf{R} = \frac{m_1 \mathbf{r}_1 + m_2 \mathbf{r}_2}{m}, \quad \mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2 \quad \text{and} \quad \mathbf{P} = \mathbf{p}_1 + \mathbf{p}_2, \quad \mathbf{p} = \mathbf{p}_1 - \mathbf{p}_2, \quad (1)$$

where  $m = m_1 + m_2$  is a total mass of the system, we can separate the decoupled center-of-mass from the relative motion in configuration or momentum space. In these coordinates, the nontrivial motion of

the system of two particles occurs entirely in the reduced problem of one body motion and motion of the center-of-mass. The total Hamiltonian of the system can be presented as a sum of two parts. One part describes the motion of the center-of-mass while the other two particles relative motion:  $H = \frac{\mathbf{P}^2}{2m} + H_r$  with  $H_r = \frac{\mathbf{p}^2}{2\mu} + V(r)$ , where  $\mu = m_1 m_2 / m$  is two body's reduced mass. The Hamiltonian  $H_r$  governs the relative motion of two particles and, when the Schrödinger equation with this Hamiltonian have been solved, the wave function of the relative motion of two particles is obtained.

Today graphene has been attracting a great deal of experimental and theoretical attention because of unusual properties in its band structure [17, 18]. Graphene is a two-dimensional layer of carbon atoms, where the atoms form honeycomb lattice [19, 20]. In the low-energy limit the low energy excitations in graphene are described not by the Schrödinger equation but instead in graphene electron and holes behave as relativistic massless particles described by a Dirac-like equation for massless and chiral particles [21–25], which is known as Weyl equation. Many of the unusual properties of graphene arise from the fact that its quasiparticles are described by Dirac spinors. Since electron and holes in graphene are governed by the Weyl equation they have an intrinsic degree of freedom that resembles the spin degree of freedom in the original Weyl equation. This degree of freedom is called pseudospin in order to distinguish it from the spin and is described by the Pauli matrices. In connection to the pseudospin, there is a good quantum number - the chirality that is defined to be the projection of the 2-momentum operator on the direction of the pseudospin. Clearly, the electrons will have positive chirality and the holes will have negative chirality. Also the Fermi speed  $v_F \sim 10^6$  m/s that is around 300 times slower than speed of light replaces the speed of light in the original Weyl equation. The positive-energy solutions of this 2D equation describes electrons, whereas the negative-energy solutions describes holes.

A 2D exciton which is a bound state of an interacting electron and hole in gapped graphene presents a two-body system and it is a fundamental and practical interest to focus on solution of two-body problem in graphene. Graphene consists of two equivalent carbon sublattices and quantum-mechanical hopping between the sublattices leads to the formation of two energy bands, and their intersection near the edges of the Brillouin zone yields the conical energy spectrum. As a result, quasiparticles in graphene exhibit a linear dispersion relation. The formation of excitons requires the existence of the energy gap in electron and hole energy spectrum. The formation of excitons in gapped graphene was studied in Refs. [12, 26–28]. The electronic ground state of intrinsic graphene and bilayer graphene in the absence of the energy gap using density functional theory within the local-density approximation and Bethe-Salpeter equation was studied in Ref. [29]. According to Ref. [29], no pure bound exciton was identified in intrinsic graphene and bilayer graphene in the absence of the energy gap. Therefore, excitons in graphene can be formed due to an energy gap opening in the electron and hole spectra in the graphene layer. There are different mechanisms of electronic excitations in graphene. The energy gap in graphene can be induced and controlled by a magnetic field, doping, an electric field in biased graphene, and hydrogenation [26, 30–32].

By contrast quantum mechanics in the description of relativistic two-body problem the situation is extremely more complicated and till now there is no completely self-consistent theory for the separation of the center-of-mass and relative motions even for the two-body case. This is due to the following facts:

- i) the particles locations and momenta are 4-vectors,
- ii) the momenta are not independent but must satisfy mass-shell conditions,
- iii) the inter-particle interaction potentials appear in the boosts as well as in the energy generator in the instant form of dynamics. As a result of a transformation to the center-of-mass system even a scalar action-at-a-distance inter-particle interaction potential becomes dependent on a coordinate and momentum.

- iv) the structure of the Poincare' group implies that there is no definition of relativistic 4-center of mass sharing all the properties of the non-relativistic 3-center of mass [33].

The two body problem in graphene when the electron and hole are interacted via a scalar action-at-a-distance inter-particle potential and are described by Weyl's equation becomes even more complicated than in simple relativistic case. Firstly, it is related to the fact that speed of light in the Weyl equation for graphene is replaced by the the Fermi speed and the resultant equation becomes non-covariant and canonical transformation implementing the separation of the center-of-mass from the relative variables within relativistic approach is invalidated. Secondly, even the inter-particle interaction depends only on the coordinate of the relative motion after to the center-of-mass transformation it becomes dependent also on a momentum. Lastly, the center-of-mass energy can not be separated from the relative motion even though the interaction depends only on the coordinate of the relative motion. This is caused by the chiral nature of Dirac electron in graphene.

Our paper is organized in the following way. In Sec. II we present the Hamiltonian of the spatially separated electron and hole in two different parallel graphene layers separated by a dielectric in the presence of the band gap. In Sec. III is given the procedure of separation of the center-of-mass and relative motions for two particles in graphene. In Sec. IV we obtain the energy spectrum and wave function of dipole exciton in two-layers graphene and find the effective exciton mass. The energy spectrum and wave function of exciton formed in a gapped graphene layer and corresponding effective exciton mass are given in Sec. V. Finally, the conclusions follow in Sec. VI.

## II. EXCITON HAMILTONIAN

Let us consider two different parallel graphene layers with the interlayer separation  $D$  and assume that excitons in this system are formed by the electrons located in the one graphene layer and, correspondingly, the holes located in the other. In this system electrons and holes move in two separate layers with honeycomb lattice structure. Since the motion of the electron is restricted in one graphene layer and the motion of the hole is restricted in the other graphene layer, we replace the coordinate vectors of the electron and hole by their projections  $\mathbf{r}_1$  and  $\mathbf{r}_2$  on plane of one of the graphene sheet. These new in-plane coordinates  $\mathbf{r}_1$  and  $\mathbf{r}_2$  will be used everywhere below. Thus, we reduced the restricted 3D two-body problem to the 2D two-body problem on the graphene plane. Each honeycomb lattice is characterized by the coordinates  $(\mathbf{r}_j, 1)$  on sublattice A and  $(\mathbf{r}_j, 2)$  on sublattice B with  $j = 1, 2$  referring to the two sheets. Then the two-particle wave function, describing two particles in different sheets, reads  $\Psi(\mathbf{r}_1, s_1; \mathbf{r}_2, s_2)$ , where  $\mathbf{r}_1$  and  $\mathbf{r}_2$  represent the coordinates of the electron and hole, correspondingly, and  $s_1, s_2$  are sublattice indices. This wave function can also be understood as a four-component spinor, where the spinor components refer to the four possible values of the sublattice indices  $s_1, s_2$ :

$$\Psi(\mathbf{r}_1, s_1; \mathbf{r}_2, s_2) = \begin{pmatrix} \phi_{aa}(\mathbf{r}_1, \mathbf{r}_2) \\ \phi_{ab}(\mathbf{r}_1, \mathbf{r}_2) \\ \phi_{ba}(\mathbf{r}_1, \mathbf{r}_2) \\ \phi_{bb}(\mathbf{r}_1, \mathbf{r}_2) \end{pmatrix} \equiv \begin{pmatrix} \Psi_a \\ \Psi_b \end{pmatrix}, \text{ where } \Psi_a = \begin{pmatrix} \phi_{aa} \\ \phi_{ab} \end{pmatrix}, \quad \Psi_b = \begin{pmatrix} \phi_{ba} \\ \phi_{bb} \end{pmatrix}. \quad (2)$$

The two components mean that one particle is on sublattice a(b) and the other particle is on sublattice a(b), correspondingly. In other words, the spinor components are from the same tight-binding wave function at different sites. Each graphene layer has an energy gap. Obviously the energy gaps in graphene layers are independent and in the general case we can introduce two non-equal gaps  $\delta_1$  and  $\delta_2$  for the first and the second graphene layers, respectively.

The corresponding hopping matrix for two non-interacting particles, including the energy gaps  $\delta_1$  and  $\delta_2$  on the first and second layers, correspondingly, then reads

$$\mathcal{H}_0 = \begin{pmatrix} -\delta_1 + \delta_2 & d_2 & d_1 & 0 \\ d_2^\dagger & -\delta_1 - \delta_2 & 0 & d_1 \\ d_1^\dagger & 0 & \delta_1 + \delta_2 & d_2 \\ 0 & d_1^\dagger & d_2^\dagger & \delta_1 - \delta_2 \end{pmatrix}. \quad (3)$$

In Eq. (3)  $d_1 = \hbar v_F(-i\partial_{x_1} - \partial_{y_1})$ ,  $d_2 = \hbar v_F(-i\partial_{x_2} - \partial_{y_2})$  and the corresponding hermitian conjugates are  $d_1^\dagger = \hbar v_F(-i\partial_{x_1} + \partial_{y_1})$ ,  $d_2^\dagger = \hbar v_F(-i\partial_{x_2} + \partial_{y_2})$ , where  $\partial_x = \partial/\partial x$  and  $\partial_y = \partial/\partial y$ ,  $x_1, y_1$  and  $x_2, y_2$  are the coordinates of vectors  $\mathbf{r}_1$  and  $\mathbf{r}_2$ , correspondingly, and  $v_F$  is the Fermi velocity of electrons in graphene. This Hamiltonian allows us to write the eigenvalue equation for two non-interacting particles as

$$\mathcal{H}_0 \Psi_0 = \epsilon_0 \Psi_0, \quad (4)$$

which leads to the following eigenenergies:

$$\epsilon_0(k_1, \delta_1; k_2, \delta_2) = \pm \sqrt{\hbar^2 k_1^2 + \hbar^2 k_2^2 + \delta_1^2 + \delta_2^2 \pm 2\sqrt{(\hbar^2 k_1^2 + \delta_1^2)(\hbar^2 k_2^2 + \delta_2^2)}} = \pm \sqrt{\hbar^2 k_1^2 + \delta_1^2} \pm \sqrt{\hbar^2 k_2^2 + \delta_2^2}. \quad (5)$$

where  $k_1$  and  $k_2$  are momentum of each particle, correspondingly. Eq. (5) gives the energy spectrum for two non-interacting particles in the presents of the non-equal gaps energies  $\delta_1$  and  $\delta_2$ . The energy

dispersion is symmetrical with respect to the replacement of particles 1 and 2. When there are no gaps,  $\delta_1 = 0$  and  $\delta_2 = 0$ , as it follows from (5) the energy dispersion is  $\pm \hbar k_1 \pm \hbar k_2$ .

Let's consider the electron and hole located in two graphene sheets with the interlayer separation  $D$ , and interacting via the Coulomb potential  $V(r)$ , where  $r$  is the projection of the distance between an electron and a hole on the plane parallel to the graphene layers. Now the problem for the two interacting particles located in different graphene layers with the broken sublattice symmetry in each layer can be described by the Hamiltonian

$$\mathcal{H} = \begin{pmatrix} -\delta_1 + \delta_2 + V(r) & d_2 & d_1 & 0 \\ d_2^\dagger & -\delta_1 - \delta_2 + V(r) & 0 & d_1 \\ d_1^\dagger & 0 & \delta_1 + \delta_2 + V(r) & d_2 \\ 0 & d_1^\dagger & d_2^\dagger & \delta_1 - \delta_2 + V(r) \end{pmatrix}, \quad (6)$$

and the eigenvalue problem for Hamiltonian (6) is

$$\mathcal{H}\Psi = \epsilon\Psi, \quad (7)$$

where  $\Psi$  are four-component eigenfunctions as given in Eq.(2).

The Hamiltonian (6) describes two interacting particles located in two graphene layers and satisfies the following conditions:

- i) when both gaps vanish  $\delta_1 = 0$  and  $\delta_2 = 0$ , as well as two-body potential  $V(r) = 0$ , the Hamiltonian describes two non-interacting Dirac particles. It is important to mention that eigenenergies are symmetrical with respect to the replacement of particle 1 and 2.
- ii) when the interaction between particles vanishes,  $V(r) = 0$ , it describes two independent particles, each located in the separate graphene layer, having two independent gaps energies related to the broken sublattice symmetry in each graphene sheet;
- iii) when the gaps in each graphene layer vanish,  $\delta_1 = 0$  and  $\delta_2 = 0$ , the Hamiltonian describes two interacting particles in one graphene layer interacting via Coulomb potential  $V(r)$  and is identical to the Hamiltonian (2) in Ref. [27] representing the two-body problem in one graphene layer if the band gap is absent;
- iv) when the gaps  $\delta_1 = \delta_2 \equiv \delta$ , the Hamiltonian describes two interacting particles in one graphene layer interacting via Coulomb potential  $V(r) = e^2/4\pi\epsilon_0\epsilon r$ , where  $e$  is the charge of the electron and  $\epsilon$  is the dielectric constant of the graphene layer.
- v) when an electron and hole located in two different graphene sheets with the interlayer separation  $D$ , they interacting via the potential  $V(r) = -e^2/4\pi\epsilon_0\epsilon_d\sqrt{r^2 + D^2}$ , where  $\epsilon_d$  is the dielectric constant of the dielectric between two graphene layers. Let us mention that for  $\delta_1 = \delta_2 = 0$  and  $D = 0$  the Hamiltonian (6) is also identical to the Hamiltonian (2) in Ref. [27].

### III. SEPARATION OF THE CENTER-OF-MASS AND RELATIVE MOTIONS

In Hamiltonian (6) the center-of-mass energy can not be separated from the relative motion even though the interaction  $V = V(r)$  depends only on the coordinate of the relative motion. This is caused by the chiral nature of Dirac electron in graphene. The similar conclusion was made for the two-particle problem in graphene in Ref. [27].

Since the electron-hole Coulomb interaction depends only on the relative coordinate, we introduce the new “center-of-mass” coordinates in the plane of a graphene sheet:

$$\begin{aligned} \mathbf{R} &= \alpha\mathbf{r}_1 + \beta\mathbf{r}_2, \\ \mathbf{r} &= \mathbf{r}_1 - \mathbf{r}_2. \end{aligned} \quad (8)$$

Here the coefficients  $\alpha$  and  $\beta$  are to be determined later. Apparently we can use the analogy of the two-particle problem for Dirac particles in gapped two-layer graphene with the center-of-mass coordinates for the case of Schrödinger equation. The coefficients  $\alpha$  and  $\beta$  will be found below from the condition of the separation of the coordinates of the center-of-mass and relative motion in the Hamiltonian in the one-dimensional “scalar” equation determining the corresponding component of the wave function.

To find the solution of (7) we make Anzätze

$$\Psi_j(\mathbf{R}, \mathbf{r}) = e^{i\mathbf{K} \cdot \mathbf{R}} \psi_j(\mathbf{r}) . \quad (9)$$

Let us introduce the following notations:

$$\begin{aligned} \mathcal{K}_+ &= \mathcal{K} e^{i\Theta} = \mathcal{K}_x + i\mathcal{K}_y , \\ \mathcal{K}_- &= \mathcal{K} e^{-i\Theta} = \mathcal{K}_x - i\mathcal{K}_y , \\ \Theta &= \tan^{-1} \left( \frac{\mathcal{K}_y}{\mathcal{K}_x} \right) , \end{aligned} \quad (10)$$

and rewrite the Hamiltonian (6) in terms of the representation of the coordinates  $\mathbf{R}$  and  $\mathbf{r}$  in a form of the  $2 \times 2$  matrix as

$$\mathcal{H} = \begin{pmatrix} \mathcal{O}_2 + V(r)\sigma_0 - \delta_1\sigma_0 + \delta_2\sigma_3 & \mathcal{O}_1 \\ \mathcal{O}_1^\dagger & \mathcal{O}_2 + V(r)\sigma_0 - \delta_1\sigma_0 + \delta_2\sigma_3 \end{pmatrix} , \quad (11)$$

where  $\mathcal{O}_1$  and  $\mathcal{O}_2$  are given by

$$\mathcal{O}_1 = \hbar v_F (\alpha \mathcal{K}_- - i\partial_x - \partial_y) \sigma_0, \quad (12)$$

$$\mathcal{O}_2 = \hbar v_F \begin{pmatrix} 0 & \beta \mathcal{K}_- + i\partial_x + \partial_y \\ \beta \mathcal{K}_+ + i\partial_x - \partial_y & 0 \end{pmatrix} \quad (13)$$

where  $x$  and  $y$  are the components of vector  $\mathbf{r}$ ,  $\sigma_j$  are the Pauli matrices,  $\sigma_0$  is the  $2 \times 2$  unit matrix. Analysis of the operators (12) and (13) shows that the coordinates of the center-of-mass and relative motion can be separated in a certain approximation.

For the Hamiltonian (11) the eigenvalue problem  $\mathcal{H}\Psi = \epsilon\Psi$  results in the following equations:

$$\begin{aligned} (\mathcal{O}_2 + V(r)\sigma_0 - \delta_1\sigma_0 + \delta_2\sigma_3) \Psi_a + \mathcal{O}_1 \Psi_b &= \epsilon \sigma_0 \Psi_a \\ \mathcal{O}_1^\dagger \Psi_a + (\mathcal{O}_2 + V(r)\sigma_0 - \delta_1\sigma_0 + \delta_2\sigma_3) \Psi_b &= \epsilon \sigma_0 \Psi_b . \end{aligned} \quad (14)$$

From Eq. (14) we have:

$$\Psi_b = (\epsilon \sigma_0 - \mathcal{O}_2 - V(r)\sigma_0 + \delta_1\sigma_0 - \delta_2\sigma_3)^{-1} \mathcal{O}_1^\dagger \Psi_a . \quad (15)$$

Assuming the interaction potential and both relative and center-of-mass kinetic energies are small compared to the gaps  $\delta_1$  and  $\delta_2$  we use the following approximation:

$$(\epsilon \sigma_0 - \mathcal{O}_2 - V(r)\sigma_0 + \delta_1\sigma_0 - \delta_2\sigma_3)^{-1} \simeq \frac{1}{\epsilon \sigma_0 + \delta_1\sigma_0 - \delta_2\sigma_3} . \quad (16)$$

Using the fact that the operator  $\mathcal{O}_1^\dagger \mathcal{O}_1$  is purely hermitian, applying Eq. (14) and

$$\mathcal{O}_1^\dagger \mathcal{O}_1 = \hbar^2 v_F^2 (\alpha^2 \mathcal{K}^2 - \nabla_{\mathbf{r}}^2 - 2i\alpha(\mathcal{K}_x \partial_y + \mathcal{K}_y \partial_x)) \sigma_0 , \quad (17)$$

we obtain:

$$(\mathcal{O}_2 + V(r)\sigma_0 - \delta_1\sigma_0 + \delta_2\sigma_3) \Psi_a + \hbar^2 v_F^2 \frac{(\alpha^2 \mathcal{K}^2 - \nabla_{\mathbf{r}}^2 - 2i\alpha(\mathcal{K}_x \partial_x + \mathcal{K}_y \partial_y))}{\epsilon \sigma_0 + \delta_1\sigma_0 - \delta_2\sigma_3} \Psi_a = \epsilon \sigma_0 \Psi_a . \quad (18)$$

Now using Eq. (2) we rewrite Eq. (18) for the individual spinor components in the following form:

$$\begin{aligned} &\left( -\delta_1 + \delta_2 + V(r) + \hbar^2 v_F^2 \frac{\alpha^2 \mathcal{K}^2 - \nabla_{\mathbf{r}}^2 - 2i\hbar v_F \alpha (\mathcal{K}_x \partial_x + \mathcal{K}_y \partial_y)}{\epsilon - \delta_1 - \delta_2} \right) \phi_{aa} + \\ &\hbar v_F (\beta \mathcal{K}_- + i\partial_x + \partial_y) \phi_{ab} = \epsilon \phi_{aa} , \end{aligned} \quad (19)$$

$$\begin{aligned} &\hbar v_F (\beta \mathcal{K}_+ + i\partial_x - \partial_y) \phi_{aa} + \\ &\left( -\delta_1 - \delta_2 + V(r) + \hbar^2 v_F^2 \frac{\alpha^2 \mathcal{K}^2 - \nabla_{\mathbf{r}}^2 - 2i\alpha(\mathcal{K}_x \partial_x + \mathcal{K}_y \partial_y)}{\epsilon - \delta_1 + \delta_2} \right) \phi_{ab} = \epsilon \phi_{ab} . \end{aligned} \quad (20)$$

We solve Eq. (20) with respect to  $\phi_{ab}$ :

$$\phi_{ab} = \left[ \epsilon + \delta_1 + \delta_2 - V(r) - \hbar^2 v_F^2 \frac{\alpha^2 \mathcal{K}^2 - \nabla_{\mathbf{r}}^2 - 2i\alpha(\mathcal{K}_x \partial_x + \mathcal{K}_y \partial_y)}{\epsilon - \delta_1 + \delta_2} \right]^{-1} (\beta \mathcal{K}_+ + i\partial_x - \partial_y) \hbar v_F \phi_{aa} . \quad (21)$$

Substituting  $\phi_{ab}$  from Eq. (21) into Eq. (19), we obtain:

$$\begin{aligned} & \left( -\delta_1 + \delta_2 + V(r) + \hbar^2 v_F^2 \frac{\alpha^2 \mathcal{K}^2 - \nabla_{\mathbf{r}}^2 - 2i\alpha(\mathcal{K}_x \partial_x + \mathcal{K}_y \partial_y)}{\epsilon - \delta_1 - \delta_2} \right) \phi_{aa} + \\ & + \hbar^2 v_F^2 (\beta \mathcal{K}_- + i\partial_x + \partial_y) \left[ \epsilon + \delta_1 + \delta_2 - V(r) - \hbar^2 v_F^2 \frac{\alpha^2 \mathcal{K}^2 - \nabla_{\mathbf{r}}^2 - 2i\alpha(\mathcal{K}_x \partial_x + \mathcal{K}_y \partial_y)}{\epsilon - \delta_1 + \delta_2} \right]^{-1} \\ & \times (\beta \mathcal{K}_+ + i\partial_x - \partial_y) = \epsilon \phi_{aa} . \end{aligned} \quad (22)$$

Assuming again that the interaction potential and both relative and center-of-mass kinetic energies are small compared to the gaps  $\delta_1$  and  $\delta_2$  we apply to Eq. (22) the following approximation:

$$\left[ \epsilon + \delta_1 + \delta_2 - V(r) - \hbar^2 v_F^2 \frac{\alpha^2 \mathcal{K}^2 - \nabla_{\mathbf{r}}^2 - 2i\alpha(\mathcal{K}_x \partial_x + \mathcal{K}_y \partial_y)}{\epsilon - \delta_1 + \delta_2} \right]^{-1} = \frac{1}{\epsilon + \delta_1 + \delta_2} . \quad (23)$$

Applying the approximation given by Eq. (23) to Eq. (22), we get from Eq. (22) the eigenvalue equation spinor component  $\phi_{aa}$  in the form:

$$\begin{aligned} & \left( -\delta_1 + \delta_2 + V(r) + \hbar^2 v_F^2 \frac{\alpha^2 \mathcal{K}^2 - \nabla_{\mathbf{r}}^2 - 2i\alpha(\mathcal{K}_x \partial_x + \mathcal{K}_y \partial_y)}{\epsilon - \delta_1 - \delta_2} \right. \\ & \left. + \hbar^2 v_F^2 \frac{\beta^2 \mathcal{K}^2 - \nabla_{\mathbf{r}}^2 - 2i\beta(\mathcal{K}_x \partial_x + \mathcal{K}_y \partial_y)}{\epsilon - \delta_1 - \delta_2} \right) \phi_{aa} = \epsilon \phi_{aa} . \end{aligned} \quad (24)$$

Choosing the values for the coefficients  $\alpha$  and  $\beta$  to separate the coordinates of the center-of-mass (the wave vector  $\mathcal{K}$ ) and relative motion  $\mathbf{r}$  in Eq. (24), we have

$$\begin{aligned} \alpha &= \frac{\epsilon - \delta_1 - \delta_2}{2\epsilon} , \\ \beta &= \frac{\epsilon + \delta_1 + \delta_2}{2\epsilon} . \end{aligned} \quad (25)$$

After substitution of Eq. (25) into Eq. (24) we can obtain the component  $\phi_{aa}$  of the spinor (2) as a solution of one-dimensional second order differential equation:

$$\left( \frac{(\hbar v_F \mathcal{K})^2}{2\epsilon} + V(r) - \frac{\epsilon(\hbar v_F)^2 \nabla_{\mathbf{r}}^2}{2(\epsilon^2 - (\delta_1 + \delta_2)^2)} \right) \phi_{aa} = [\epsilon + \delta_1 - \delta_2] \phi_{aa} . \quad (26)$$

The other components of (2) can be found as:

$$\Psi_b = -(\epsilon \sigma_0 + (\partial_{x_2} \sigma_1 - i\partial_{y_2} \sigma_2) - \delta_1 \sigma_0 - \delta_2 \sigma_3 - V(r) \sigma_0)^{-1} i D_1^\dagger \Psi_a \quad (27)$$

with Pauli matrices  $\sigma_j$  and  $2 \times 2$  unit matrix  $\sigma_0$ . Moreover, we have

$$\phi_{ab} = \left[ \epsilon + \delta_1 + \delta_2 - V(r) + \frac{1}{\epsilon - \delta_1 + \delta_2} (\partial_{x_1}^2 + \partial_{y_1}^2) \right]^{-1} (i\partial_{x_2} - \partial_{y_2}) \phi_{aa} . \quad (28)$$

#### IV. TWO BODY PROBLEM IN TWO GAPPED GRAPHENE LAYERS

Let us consider an electron and hole located in two different parallel graphene layers and interacting via the potential  $V(r) = -e^2/4\pi\epsilon_0\epsilon_d\sqrt{r^2 + D^2}$ . Substituting this potential into (26) we obtain the second order differential equation for the component  $\phi_{aa}$ . This equation cannot be solved analytically. However, assuming  $r \ll D$  we can approximate  $V(r)$  by the first two terms of Taylor series and substituting  $V(r) = -V_0 + \gamma r^2$ , where  $V_0 = e^2/4\pi\epsilon_0\epsilon_d D$  and  $\gamma = e^2/8\pi\epsilon_0\epsilon_d D^3$  for the interaction potential into Eq. (26), we obtain

$$\left( -\frac{2\epsilon(\hbar v_F)^2 \nabla_{\mathbf{r}}^2}{\epsilon^2 - (\delta_1 + \delta_2)^2} + \gamma r^2 \right) \phi_{aa} = \left[ \epsilon + \delta_1 - \delta_2 + V_0 - \frac{(\hbar v_F \mathcal{K})^2}{2\epsilon} \right] \phi_{aa} . \quad (29)$$

The last equation can be rewritten in the form of the two-dimensional isotropic harmonic oscillator:

$$(-\mathcal{F}_1(\epsilon) \nabla_{\mathbf{r}}^2 + \gamma r^2) \phi_{aa} = \mathcal{F}_0(\epsilon) \phi_{aa} , \quad (30)$$

where

$$\begin{aligned} \mathcal{F}_1 &= \frac{2\epsilon(\hbar v_F)^2}{\epsilon^2 - (\delta_1 + \delta_2)^2} , \\ \mathcal{F}_0 &= \epsilon + \delta_1 - \delta_2 + V_0 - \frac{(\hbar v_F \mathcal{K})^2}{2\epsilon} . \end{aligned} \quad (31)$$

The eigenfunction and eigenenergy for two-dimensional isotropic parabolic well were first determined by Fock in 1928 [34], later in Ref. [35], and was studied in detail in Ref. [36]. The single-particle eigenfunction for the two-dimensional oscillator widely used for the description of quantum dot [37]. The solution of Eq. (30) is well known (see, for example, Ref. [38]) and is given by

$$\frac{\mathcal{F}_0(\epsilon)}{\mathcal{F}_1(\epsilon)} = 2N \sqrt{\frac{\gamma}{\mathcal{F}_1(\epsilon)}} ,$$

where  $N = 2\tilde{N} + |L| + 1$ , and  $\tilde{N} = \min(\tilde{n}, \tilde{n}')$ ,  $L = \tilde{n} - \tilde{n}'$ ,  $\tilde{n}, \tilde{n}' = 0, 1, 2, 3, \dots$  are the quantum numbers of the 2D harmonic oscillator. The corresponding 2D wave function in terms of associated Laguerre polynomials can be written as

$$\phi_{aa_{\tilde{N}L}}(r) = \frac{\tilde{N}!}{a^{|L|+1} \sqrt{\tilde{n}! \tilde{n}'!}} \text{sgn}(L) r^{|L|-1/2} e^{-r^2/(4a^2)} \times L_{\tilde{N}}^{|L|}(r^2/(2a^2)) \frac{e^{-iL\phi}}{(2\pi)^{1/2}} , \quad (32)$$

where  $\phi$  is the polar angle,  $L_k^p(x)$  are the associated Laguerre polynomials and  $a = \left( \sqrt{\mathcal{F}_1(\epsilon)} / (2\sqrt{\gamma}) \right)^{1/2}$ .

After some straightforward but lengthy calculations and the expansion up to second order in  $\mathcal{K}$  we obtain the following expression for the energy in quadratic order with respect to  $\mathcal{K}$

$$\epsilon = -V_0 + \sqrt{\mu^2 + \frac{C_1}{\mu}} + \frac{1}{2\mu^4} \frac{C_1}{\sqrt{1 + \frac{C_1}{\mu^3}}} (\hbar v_F \mathcal{K})^2 , \quad (33)$$

where  $\mu = \delta_1 + \delta_2$  and  $C_1 = 2\gamma N^2 (\hbar v_F)^2$ . Thus, from (33) we can conclude that the effective exciton mass  $M$  is given as a function of total energy gap  $\delta_1 + \delta_2$  as

$$M = \frac{\mu^4}{v_F^2 C_1} \sqrt{1 + \frac{C_1}{\mu^3}} . \quad (34)$$

The dependence of the effective exciton mass  $M$  defined by Eq. (34) on the total energy gap  $\delta_1 + \delta_2$  and the interlayer separation  $D$  for two graphene layers separated by the dielectric GaAs is shown in Fig. 1. Firstly, according to Fig. 1, the effective exciton mass  $M$  increases when the total energy gap  $\delta_1 + \delta_2$  and the interlayer separation  $D$  increase. Secondly, the mass increases much faster for the bigger value



of the interlayer separation and bigger value of the energy gap. Let's mentioned that the dependence of the effective exciton mass  $M$  on the interlayer separation  $D$  is caused by the quasi-relativistic Dirac Hamiltonian of the gapped electrons and holes in graphene layers. However, for the excitons in couple quantum wells (CQW) the effective exciton mass does not depend on the interlayer separation, because the electrons and holes in CQW's are described by a Schrödinger Hamiltonian, while excitons in two graphene layers are described by the Dirac-like Hamiltonian (6).

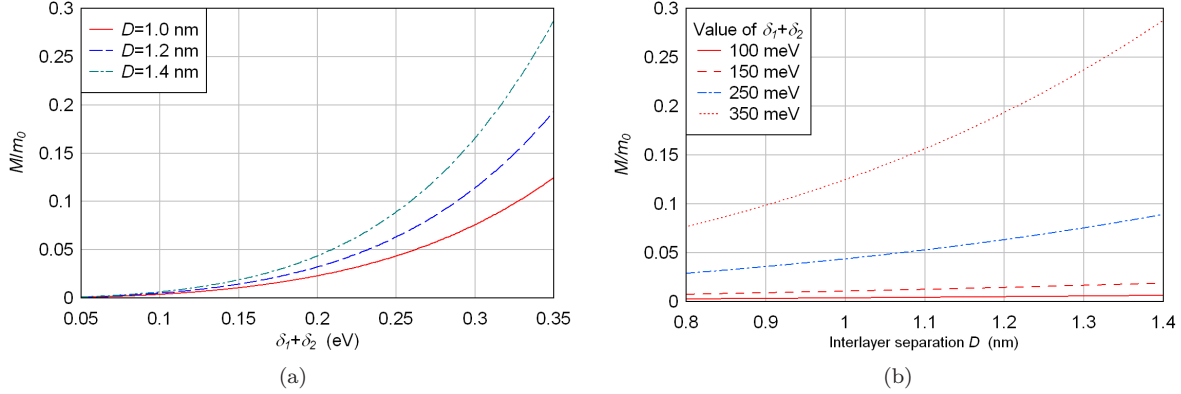


FIG. 1: Excitons in two graphene layers separated by the dielectric GaAs. The effective exciton mass  $M$  in the units of free electron mass  $m_0$  (a) as a function of the total energy gap for the different graphene interlayer separations, (b) as the function of on interlayer separation for different values of the total energy gap.

In Fig. 2 is shown the energy dispersion of exciton for different values of the total energy gap and interlayer separation and for the different dielectrics between the graphene layers. Results are presented for the parabolic approximation for the energy dispersion assuming the low-energy limit. When  $\mathcal{K} \sim 0.08 \text{ nm}^{-1}$  the parabolic approximation (33) gives about 2% difference with respect to the exact numerical solution and this percentage decreases when  $\mathcal{K}$  decreases. The analysis of the results presented in Fig. 2a shows that the energy dispersion decreases when the total energy gap increases. The same behavior can be observed for the dependence of the energy dispersion on interlayer separation: for given  $\mathcal{K}$  when interlayer separation increases the energy dispersion decreases (Fig. 2b). In Fig. 2c is given the energy dispersion of exciton for the different dielectric placed between two graphene layers. As it seen, there is small increase for the energy dispersion: for a smaller value of the dielectric constant the energy dispersion of exciton becomes bigger.

## V. TWO BODY PROBLEM IN A GAPPED GRAPHENE LAYER

Now we consider an electron and a hole located in a single gapped graphene layer with the energy gap parameter  $\delta$  and exciton formed by the electron and hole located in this graphene layer. Putting the gaps  $\delta_1 = \delta_2 \equiv \delta$  in (6), we obtain the Hamiltonian that describes two interacting particles in one graphene layer interacting via Coulomb potential  $V(r) = \frac{e^2}{4\pi\epsilon_0\epsilon r}$ . Using this potential we rewrite Eq. (26) in the form

$$\left( -\frac{2\epsilon(\hbar v_F)^2 \nabla_{\mathbf{r}}^2}{\epsilon^2 - 4\delta^2} - \frac{e^2}{4\pi\epsilon_0\epsilon r} \right) \phi_{aa} = \left[ \epsilon - \frac{(\hbar v_F \mathcal{K})^2}{2\epsilon} \right] \phi_{aa} . \quad (35)$$

Eq. (35) can be rewritten in the form of the two-dimensional hydrogen atom:

$$\left( -\mathcal{F}_1(\epsilon) \nabla_r^2 - \frac{e^2}{4\pi\epsilon_0\epsilon r} \right) \phi_{aa} = \mathcal{F}_0(\epsilon) \phi_{aa} , \quad (36)$$

where

$$\mathcal{F}_1 = \frac{2\epsilon(\hbar v_F)^2}{\epsilon^2 - 4\delta^2} , \quad \mathcal{F}_0 = \epsilon - \frac{(\hbar v_F \mathcal{K})^2}{2\epsilon} . \quad (37)$$



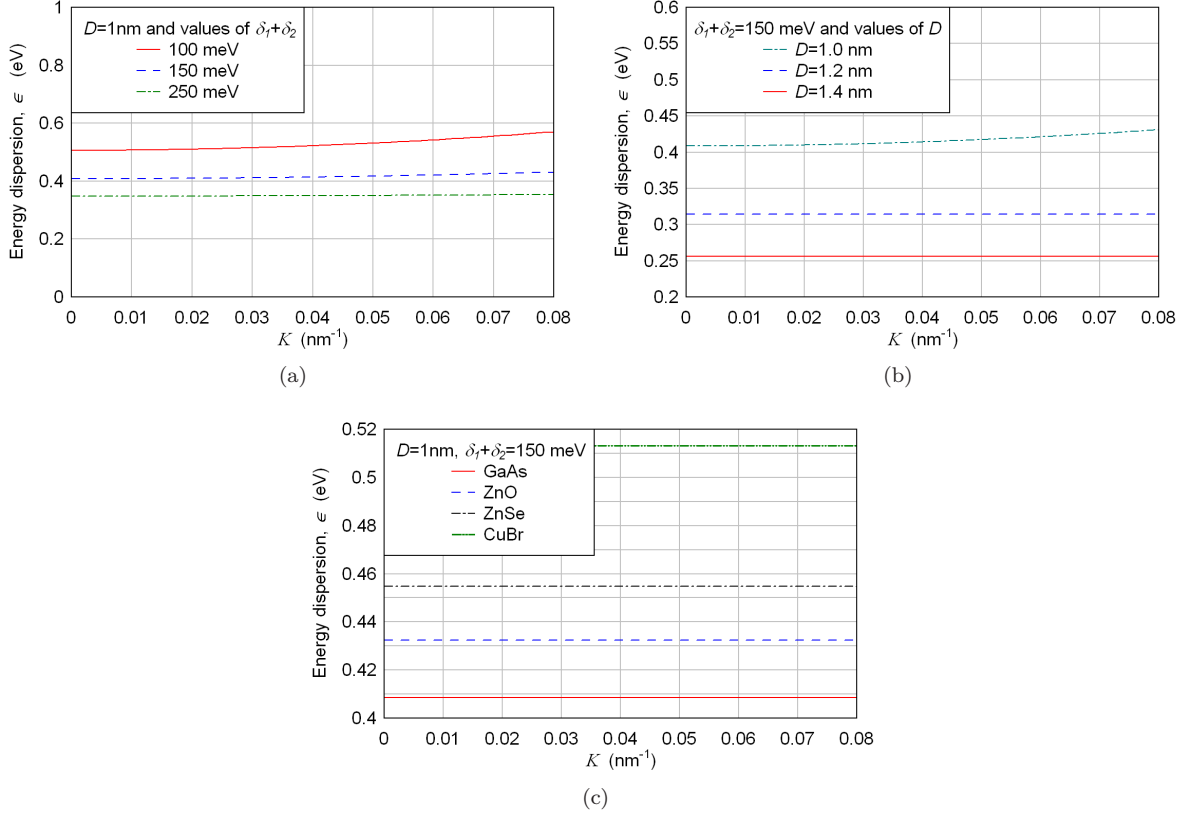


FIG. 2: Excitons in two graphene layers separated by the dielectric. The energy dispersion of exciton (a) for the fixed total energy gap and the different graphene interlayer separations, (b) for the fixed interlayer separation for different values of the total energy gap, and (c) for the fixed total energy gap, graphene interlayer separations and the different dielectrics between graphene layers.

The solution of the two-dimensional hydrogen atom equation (30) is well known [39–41] and is given by

$$\mathcal{F}_0(\epsilon) = -\frac{e^4}{4\mathcal{F}_1(\epsilon)\epsilon^2(n-1/2)^2}, \quad (38)$$

where  $n = 1, 2, 3, \dots$  are the quantum numbers, and the wave function in terms of associated Laguerre polynomials is given by

$$\phi_{aanl}(\mathbf{r}) = \tilde{\beta} \left[ \frac{(n-1-|l|)!}{[(|l|+n-1)!]^3(2n-1)} \right]^{1/2} e^{-\tilde{\beta}r/2} (\tilde{\beta}r)^{|l|} L_{n+|l|-1}^{2|l|}(\tilde{\beta}r) \frac{e^{il\varphi}}{(2\pi)^{1/2}}, \quad (39)$$

where  $\tilde{\beta} = e^2 / [(n-1/2)\epsilon\mathcal{F}_1(\epsilon)]$ ,  $\varphi$  is the polar angle,  $L_k^p(x)$  are the associated Laguerre polynomials, the quantum numbers  $l$  can take the values  $l = 0, \pm 1, \pm 2, \dots, \pm(n-1)$ .

After simplification Eq. (38) can be rewritten in the form of the following quadratic equation

$$(C + 8\gamma)\epsilon^2 - 4\gamma k^2 - 4C\delta^2 = 0, \quad (40)$$

where  $\gamma = (\hbar v_F)^2$ ,  $k = \hbar v_F \mathcal{K} = v_F P$ ,  $C = e^4 / (4\pi\epsilon_0\epsilon(n-1/2))^2$ .

The solutions of Eq. (40) are given by

$$\epsilon = 2 \left( \frac{\gamma(\hbar v_F \mathcal{K})^2 + C\delta^2}{C + 8\gamma} \right)^{1/2}. \quad (41)$$

Eq. (41) gives the energy-momentum dispersion  $\epsilon(\mathcal{K})$  of the electron and hole that are bound via Coulomb potential in a single graphene layer. Since our interest is small kinetic energy, therefore, for small  $\mathcal{K}$  we expand Eq. (41) with respect to  $\mathcal{K}^2$ : and approximate  $\epsilon(\mathcal{K})$  by the first two terms of Taylor series

$$\epsilon = E_b + \frac{(\hbar\mathcal{K})^2}{2\mathcal{M}}, \quad (42)$$

where  $E_b$  is the exciton binding energy is given by

$$E_b = 2\delta \left( \frac{C}{C + 2\gamma} \right)^{1/2}, \quad (43)$$

and  $\mathcal{M}$  is the effective mass of exciton given by

$$\mathcal{M} = \frac{\delta}{2\gamma v_F^2} \sqrt{(C + 8\gamma)C}. \quad (44)$$

We note the exciton effective mass  $\mathcal{M}$  increases when the gap  $\delta$  increases as it is shown in Fig. 3a. The result of calculation of the exciton energy dispersion in graphene layer for different gap energy  $\delta$  in low energy parabolic approximation is given in Fig. 3b. When  $\mathcal{K} \sim 0.08 \text{ nm}^{-1}$  the parabolic approximation (42) gives less than 0.5% difference with respect to the exact solution (41) and this value decreases when  $\mathcal{K}$  decreases. According to Fig. 3b, the exciton energy spectrum at the same quantum number  $n$  increases with the increase of the gap energy  $\delta$ . However, for two graphene layers separated by the dielectric the energy dispersion decreases when the total energy gap increases. Also the comparison of the exciton energy distribution in graphene layer and in two graphene layers separated by the dielectric shows that the exciton energy in graphene layer always bigger than in two graphene layers separated by the dielectric.

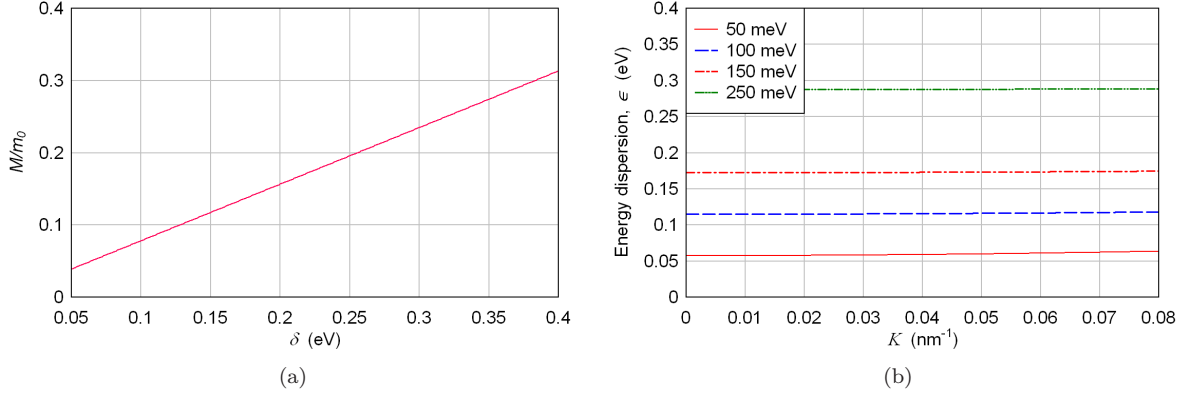


FIG. 3: Excitons in the single graphene layer. (a) The effective exciton mass as a function of the energy gap.(b) The energy dispersion of exciton for the different values of the energy gap.

## VI. CONCLUSIONS

Now let us return to the fundamental and practical question related to finding the solution of a problem of two interacting Dirac particles that form the exciton in gapped graphene layer and in two gapped graphene layers. In low-energy limit this problem can be solved analytically, and we obtained the energy dispersion and wave function of the exciton in gapped graphene layer and in two gapped graphene layers separated by a dielectric. The excitons were considered as a system of two Dirac particles interacting via a Coulomb potential  $V(r)$ . In general case the center-of-mass and can not be separated from the relative motion even though the interaction depends only on the coordinate of the relative motion. This is caused

by the chiral nature of Dirac electron in graphene and the electron and hole locations and momenta are 4-vectors and must satisfy mass-shell conditions. The analytical solution for the energy dispersion and wave function was obtained by introducing the transformation for the separation of the center-of-mass and relative motions for two particles in graphene that allows to reduce the Dirac-like equation for spinor to the Schrödinger-like second order differential equation for the component of the spinor. In the parabolic approximation for the energy dispersion found the effective mass of the exciton which are the function of the energy gap in the single graphene layer and function of the energy gaps and interlayer separation in the case of two graphene layers separated by the dielectric. Firstly, we can conclude that the exciton effective mass increases in the both cases for a single graphene layer and for two layers graphene as the gap energy increases. Also the exciton effective mass increases when the interlayer separation increases. Therefore, by tuning the energy gaps in graphene layers and changing interlayer separation one can get the desirable value for the effective exciton mass. This is very important for the system of many excitons when this system is considered as a dilute gas of excitons that forms Bose-Einstein condensate and undergoes to the Kosterlitz-Thouless phase transition to a superfluid phase. By decreasing the mass of the exciton one can increase the Kosterlitz-Thouless transition temperature. Secondly, for the exciton in graphene layer the energy dispersion increases with the increase of the gap energy. However, for the exciton in two graphene layers separated by the dielectric the energy dispersion decreases when the total energy gap increases as well as it decreases when the interlayer separation increases.

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